AMath 483/583 — Lecture 27

Outline:

- Random walk solution of Poisson problem
- Using MPI with subroutines
- Python plus Fortran: f2py

Notes and Sample codes:

- Class notes: Random numbers
- Class notes: Poisson problem
- `$UWHPSC/codes/mpi/quadrature`
- `$UWHPSC/codes/f2py`

Monte Carlo solution of Poisson problem

Suppose we want to compute an approximate solution to

$$u_{xx} + u_{yy} = 0 \qquad \text{with } u \text{ given on boundary}$$

at a single point (x_0, y_0).

Finite difference approach: Discretize domain and solve linear system for approximations U_{ij} at all points on grid.

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Do this N times and average all the values obtained.

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Instead can take a random walk starting at (x_0, y_0) and evaluate u at the first boundary point the walk reaches.

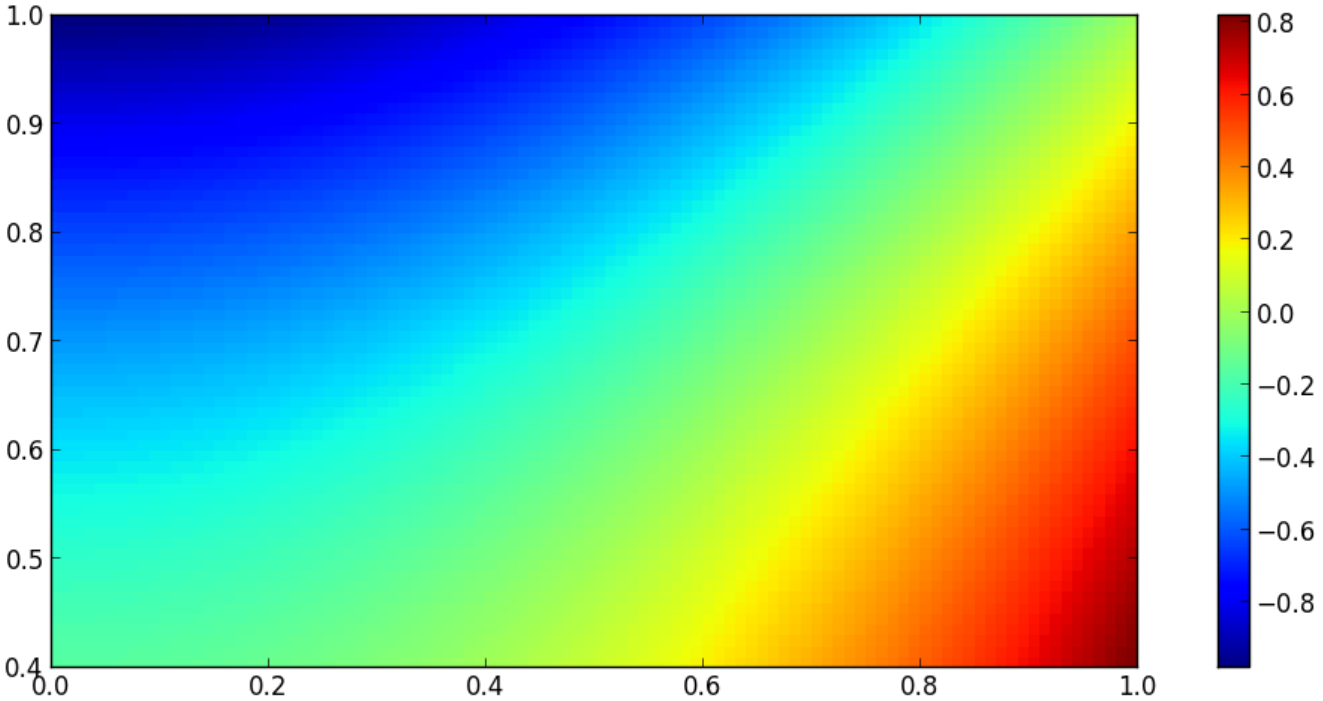
Do this N times and average all the values obtained.

This average converges to $u(x_0, y_0)$ with rate $1/\sqrt{N}$.

Monte Carlo solution of Laplace's Equation

Laplace's equation: $u_{xx}(x,y) + u_{yy}(x,y) = 0$

An exact solution: $u(x,y) = x^2 - y^2$ since $u_{xx} = 2, \quad u_{yy} = -2.$



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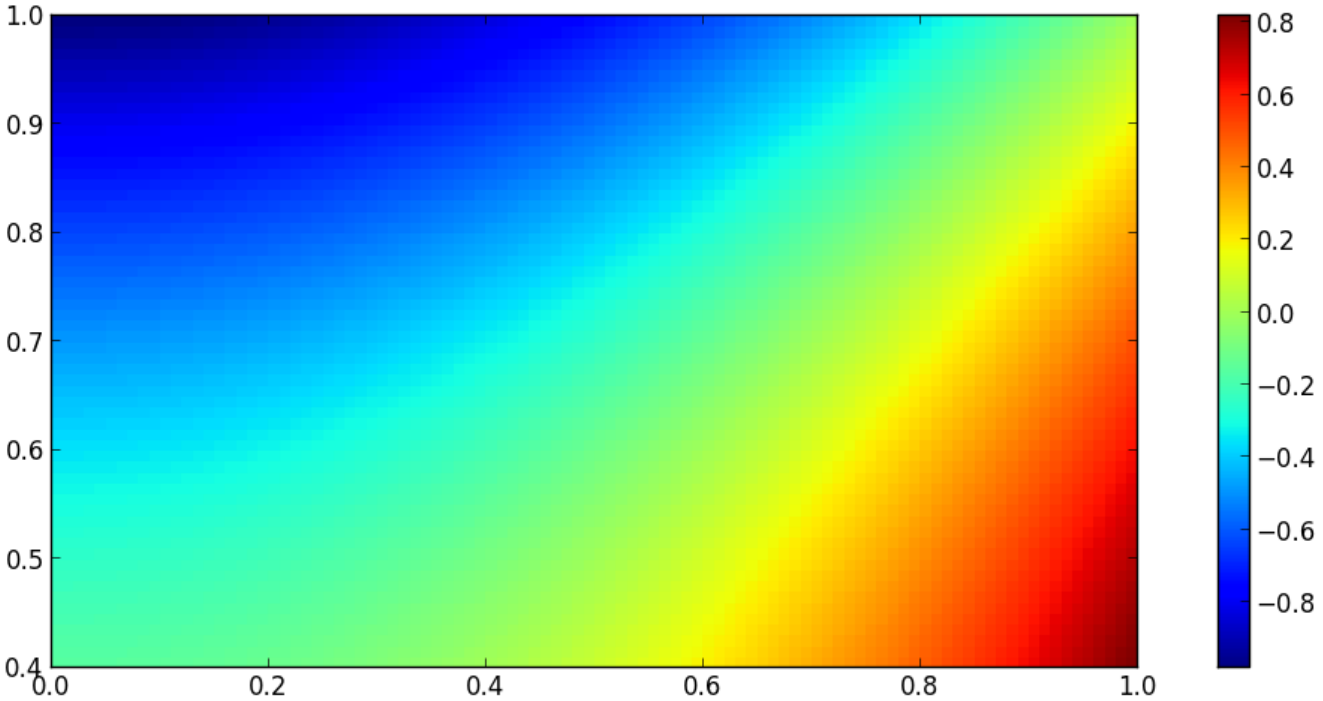
Also $U_{ij} = x_i^2 - y_j^2$ satisfies discrete equations exactly, since

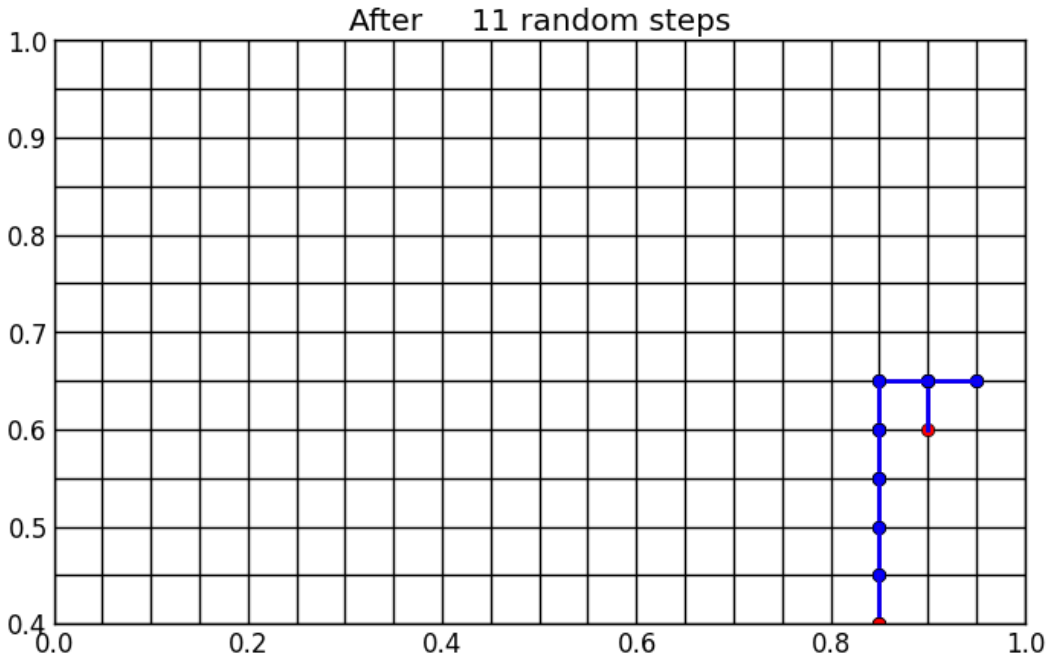
$$\frac{1}{\Delta x^2}(U_{i-1,j} - U_{ij} + U_{i+1,j}) = 2, \quad \frac{1}{\Delta y^2}(U_{i,j-1} - U_{ij} + U_{i,j+1}) = -2$$



Random walk on a lattice

$u_{xx} + u_{yy} = 0$ with solution $u(x, y) = x^2 - y^2$.

Estimate solution at $(x_0, y_0) = (0.9, 0.6)$ where $u(x_0, y_0) = 0.45$.



Hit boundary where u = 0.562500

Random walk on a lattice

Strategy:

Start at (x_0, y_0).

Each step, move to one of 4 neighbors, choosing with equal probability.

If $0 \leq r \leq 1$ is a uniformly distributed random number then decide based on:

$0 \leq r < 0.25 \implies$ move left

$0.25 \leq r < 0.5 \implies$ move right

$0.5 \leq r < 0.75 \implies$ move down

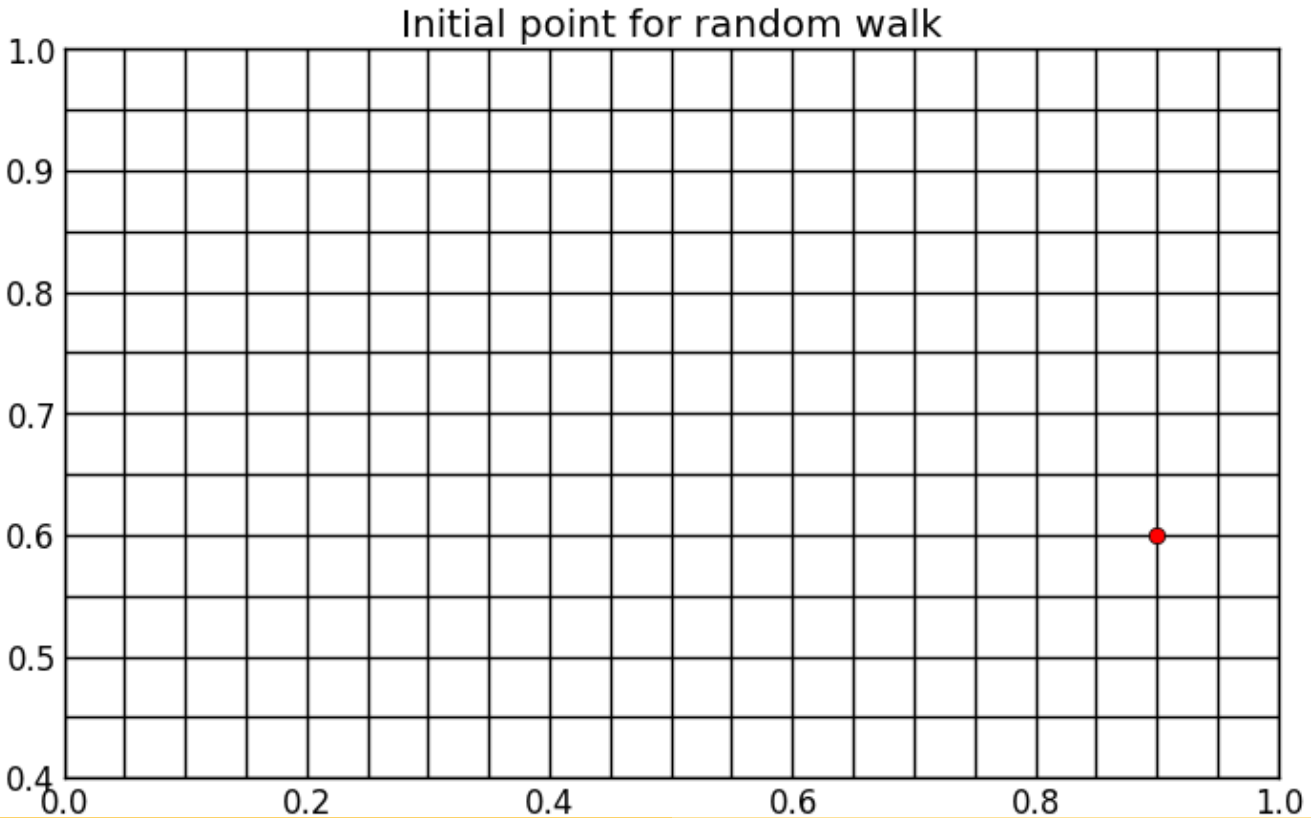
$0.75 \leq r \leq 1.0 \implies$ move down

Random walk on a lattice

Why does this work? Let E_{ij} be expected value of boundary value reached if starting at grid point (i, j).

Then $E_{ij} = \frac{1}{4}(E_{i-1,j} + E_{i+1,j} + E_{i,j-1} + E_{i,j+1})$

The same equation as finite difference method for Poisson!



MPI with subroutines and functions

Recall quadrature program from Homework 4:

In OpenMP: Subroutine is called by the single master thread running the main program

Inside the subroutine `trapezoid` a single `omp parallel` block is used to fork a set of threads that are used for the full computation.

End of a parallel block kills all threads except master thread.

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In MPI: First statement in main program must be `MPI_INIT`.

It's not possible to call `MPI_INIT` in the subroutine.

The entire code (including main program and call to subroutine) is executed by each process (maybe on different computers!).

Call to `MPI_FINALIZE` kills all processes.

MPI with subroutines and functions

MPI version of Simpson's rule program:

`$UWHPSC/codes/mpi/quadrature`

Notes:

- There is no master process except that we may decide some things should only be done by Process 0, for example.
- The module variable `gevals` is a global variable, but is still private to each process.

  All variables are private, no shared variables!

f2py — combining Fortran and Python

Often want to use

Fortran for intensive computations,

Python to provide nice user interface, plot results,

automate a series of runs with different parameters,

do convergence tests as grid size is refined, etc.

Can write data files to disk from Fortran, read into Python,

This is what we've done for plotting in homeworks.

Sometimes nice to call Fortran directly from Python.

e.g. LAPACK is used under the hood in NumPy.

f2py provides a wrapper for Fortran code.

f2py — combining Fortran and Python

Basic idea:

`fortrancode.f90` contains a function or subroutine, e.g. function `f1(x)` that returns a single value.

```
$ f2py -m mymodulename -c fortrancode.f90
```

This creates a binary file `mymodulename.so` that can used as a Python module.

```
>>> from mymodulename import f1
>>> y = f1(3.)
```

f2py — function example

$UWHPSC/codes/f2py/fcn1.f90

```
function f1(x)
    real(kind=8), intent(in) :: x
    real(kind=8) :: f1
    f1 = exp(x)
end function f1
```

Then we can do...

```
$ f2py -m fcn1 -c fcn1.f90
$ python
>>> import fcn1
>>> fcn1.f1(1.)
2.7182818284590451
```

f2py — subroutine example

$UWHPSC/codes/f2py/sub1.f90

```
    subroutine mysub(a,b,c,d)
        real (kind=8), intent(in) :: a,b
        real (kind=8), intent(out) :: c,d
        c = a+b
        d = a-b
    end subroutine mysub
```

Then we can do...

```
$ f2py -m sub1 -c sub1.f90
$ python
>>> import sub1
>>> y = sub1.mysub(3., 5.)
>>> print y
(8.0, -2.0)
```

Note: Tuple `(c, d)` is returned by the Python function.

f2py — Jacobi iteration

$UWHPSC/codes/f2py/jacobi1.f90

```
    subroutine iterate(u0,iters,f,u,n)
```

Takes input array `u0` of length `n` and right hand side array `f` and produces `u` by taking `iters` iterations of Jacobi.

$UWHPSC/codes/f2py/plot_jacobi_iterates.py

```
    # Set u = initial guess;  f = rhs
    for nn in range(nplots):
        u = jacobi1.iterate(u, iters_per_plot, f)
        plt.plot(x, u, 'o-')
        plt.draw()
        time.sleep(.5)
```

Other wrappers...

- Cython: Allows writing C code embedded in Python.
  `http://www.cython.org/`
- Jython: For Java.
  `http://www.jython.org/`
- swig: Connects C and C++ to many other languages
  `http://www.swig.org/`